Aspects of Multiscale Modeling: Kinetic Monte Carlo, Cascade Aging and Dislocation - Obstacle Interactions

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Presentation overview

- **Cascade aging objective:**

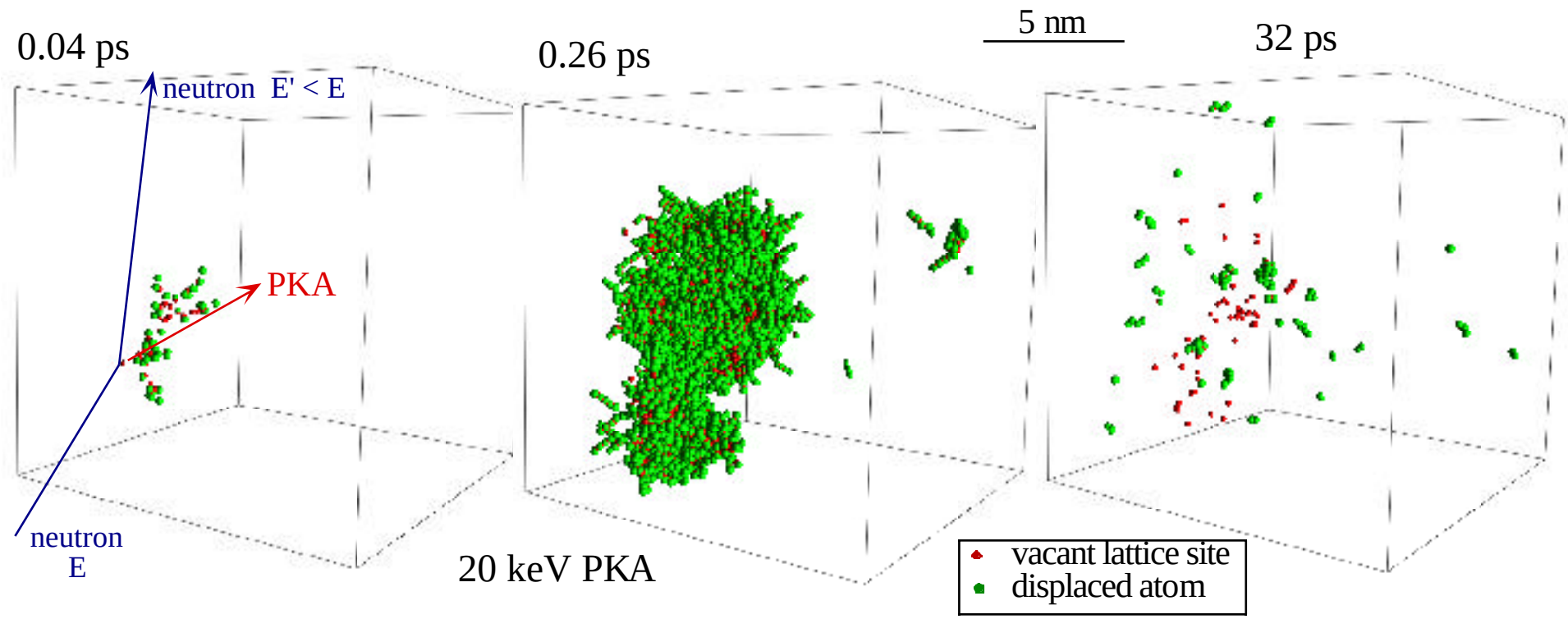
  Model the long-term defect, solute & impurity evolution

- **Kinetic Monte Carlo & cascade aging examples**

- **Molecular Dynamics/KMC model of vacancy cluster evolution & MD simulation of defect-dislocation interactions in Cu**

- **Summary of recent progress**

Objective: cascade aging

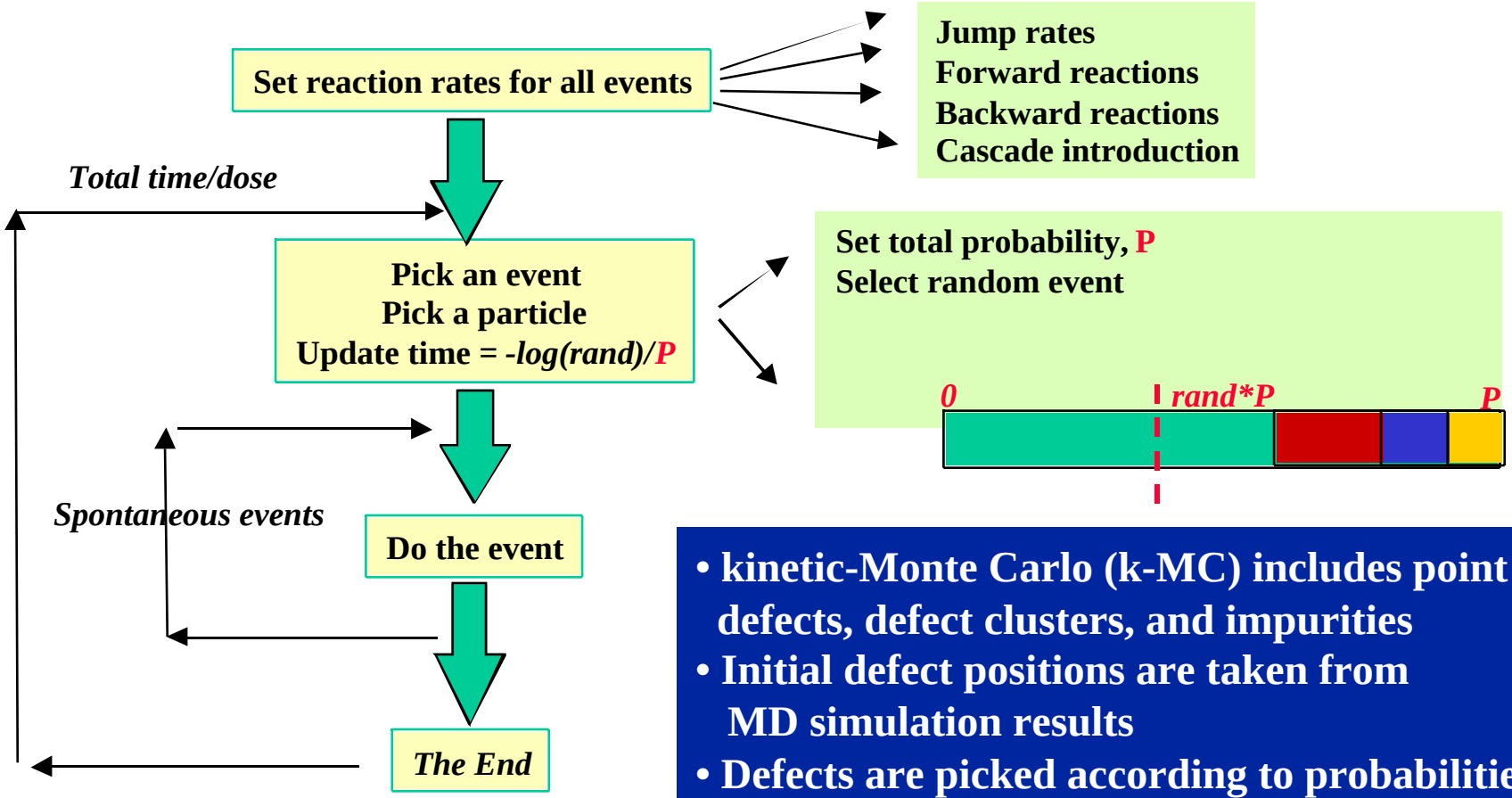


Track the fate of all defects and solutes to determine the defect/nano/microstructural features at times >> seconds

Kinetic Monte Carlo (KMC)

- **KMC: stochastic, atomic-scale model to simulate the time-evolution of defects and nano/microstructural evolution - focus on individual defects, not on atomic vibrations**
- **Probabilities/reaction rates for any given event (defect/cascade introduction, diffusion, clustering, dissolution, recombination, …) obtained from i) probability lookup tables, or ii) interatomic potentials coupled with transition state theory**
- **Events chosen at *random* - sets the timescale**
- **March forward in time**

Kinetic Monte Carlo (KMC)



- kinetic-Monte Carlo (k-MC) includes point defects, defect clusters, and impurities
- Initial defect positions are taken from MD simulation results
- Defects are picked according to probabilities based on their diffusivity:

$$P_k = \frac{N_k \nu_k}{\sum_i N_i \nu_i}$$

KMC examples

- **Intra-cascade recombination in Cu**

- **Defect-reaction kinetics (1-D diffusion)**

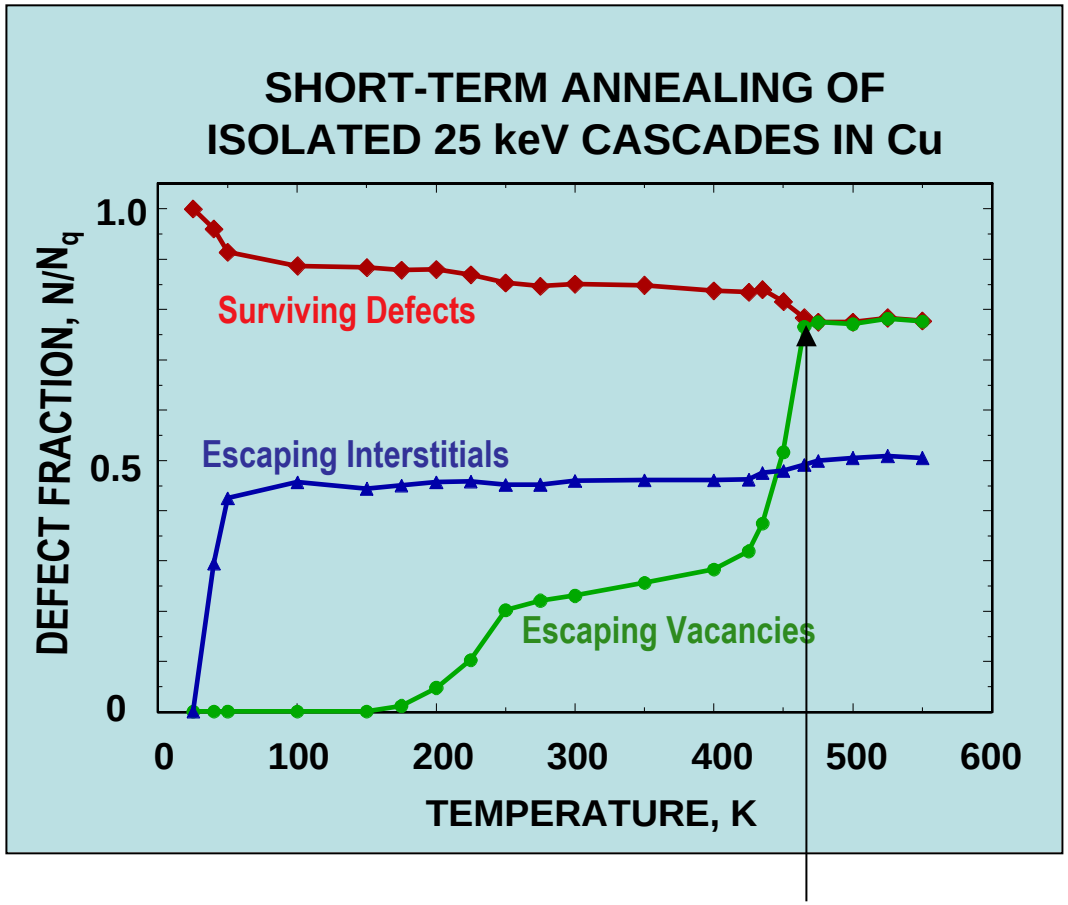
- **Vacancy cluster formation in Fe** -> link to rate theory**

  **** example from RPV embrittlement**

- **Damage accumulation in Cu (Coupled MD/KMC)**

Intra-cascade annealing in Cu

What happens to the cascade defects long after the first 10 ps?



KMC simulations of annealing individual cascade regions show the fractions of defects produced in a cascade that

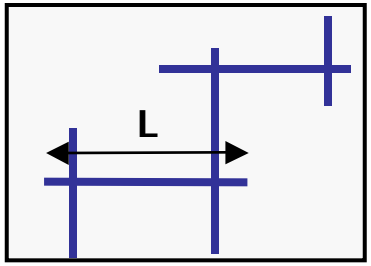
- **survive recombination**
- **escape the cascade region**
- **form stable, sessile clusters**

as a function of temperature

❖ **The large fraction of escaping vacancies at high temperatures corresponds with the experimentally observed temperature dependence of void swelling.**

Defect reaction kinetics for 1-D cluster migration

MD simulations show that SIA clusters formed in cascades migrate in 1-dimension with occasional directions changes



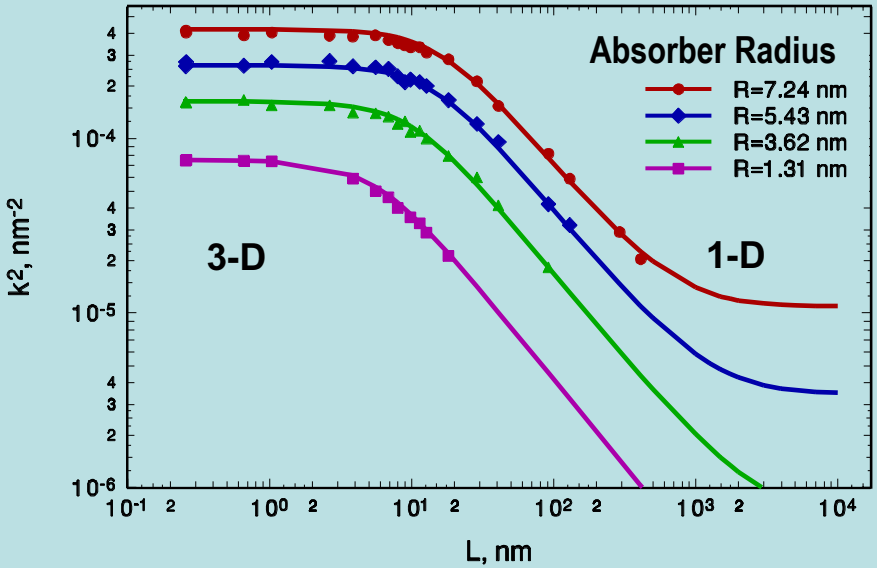
Mixed 1-D/3-D migration, average 1-D segment length L

1-D cluster migration requires a new reaction kinetics

KMC "thought experiments"

- Defects migrating by mixed 1-D/3-D with the same L, interact with …
- Random field of absorbers of radius R, number density N
- "Sink strengths" k^2 are determined from the defect lifetimes as a function of L

$$k_m^2 = 0.5\, k_1^2 \{ 1 + \sqrt{1 + 4/(l^2 k_1^2/4 + k_1^4/k_3^4)} \}$$



Sink strength as a function of 1-D segment length. Analytical expression compared to KMC results

KMC "thought experiments" are perfectly described by a new analytical theory for reaction kinetics from 1-D to 3-D.

The new reaction kinetics is incorporated into the new Production Bias Model of microstructure evolution (Singh, Woo, Trinkaus, Foreman, Golubov)

Cascade aging approach (RPV embrittlement)

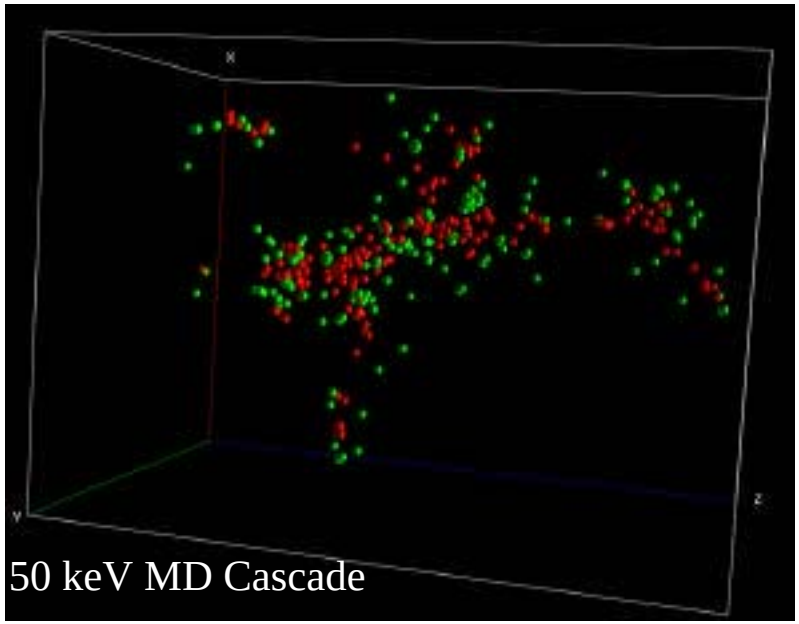
- **MD database of displacement cascade primary defect production**

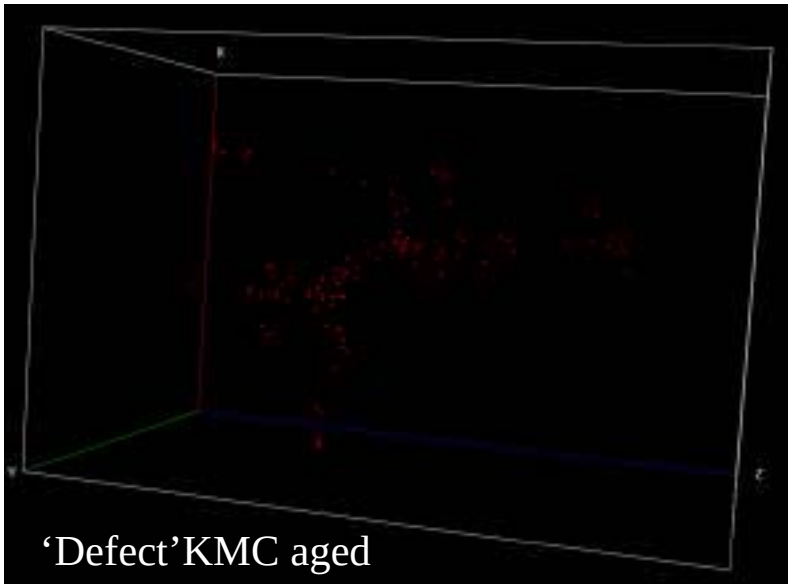
- **Short-time (~100 ns), "Defect" kinetic Monte Carlo to allow additional recombination & SIA/SIA cluster migration away from the cascade**

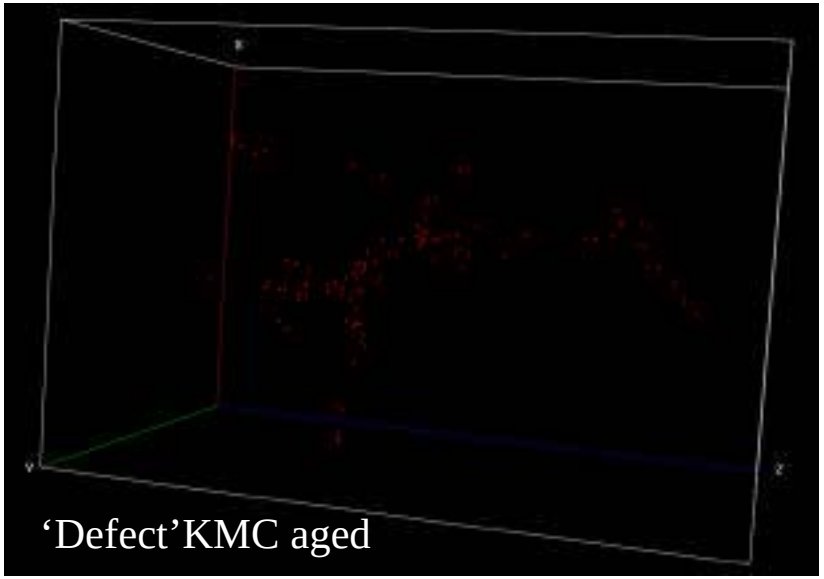
- **Kinetic lattice Monte Carlo (KLMC) using a embedded-atom method potential to track the vacancy/vacancy cluster fate**

– Generate 'long-time', *cascade-aged* defect (vacancy cluster) production cross-sections - input to rate theory

‘Defect’ KMC results - 1st 100 ns, 290°C







Cascade energy (keV)	MD defects (~ 100 ps)	Surviving vacancies (~ 100 ns)
20	54	47 (87%)
40	111	80 (72%)
50	176	111 (63%)

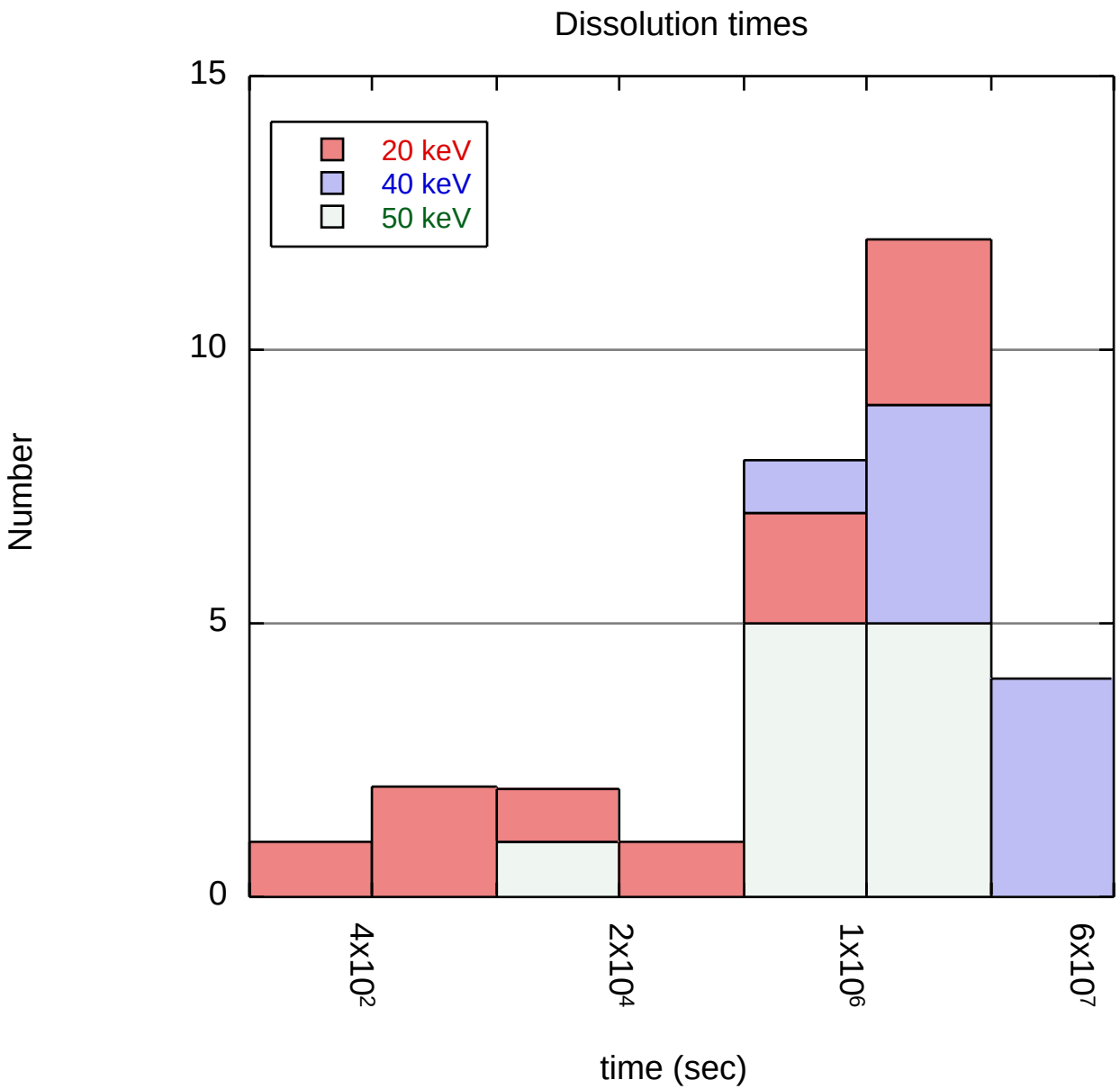
KLMC results, 50 keV cascade in Fe at 563 K

- Rapid formation of 3-D clusters

- Small clusters are mobile and cluster growth often involves coalescence

Vacancy cluster evolution movie

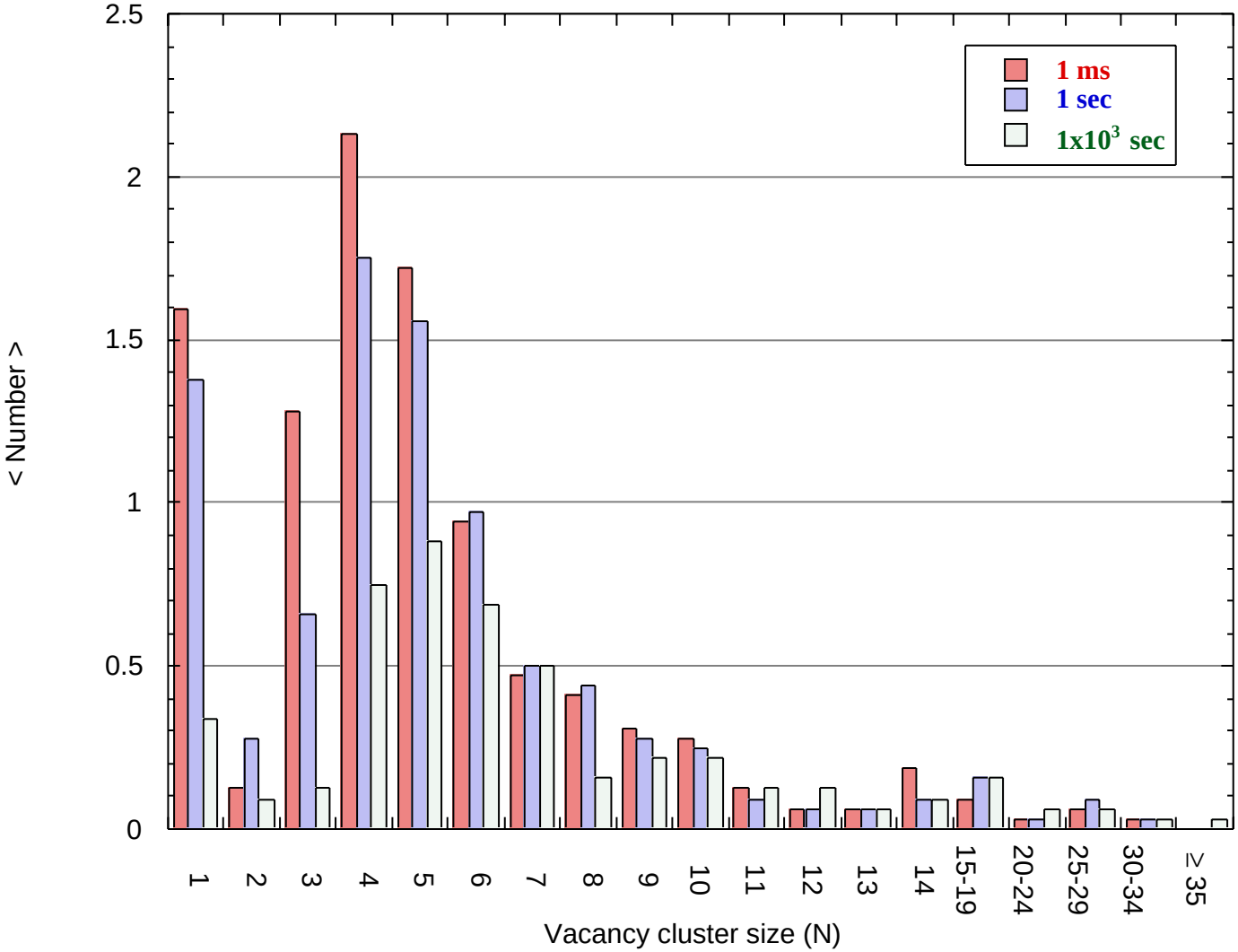
Mean vacancy cluster dissolution time



- Large number (> 40) of Cascade Aging simulations using 20, 40 & 50 keV cascades:
  - mean dissolution lifetime
  - time dependent vacancy cluster (aged) source term

Mean dissolution time ~ 4×10^5 sec

Delayed cascade vacancy cluster source term



Provide vacancy cluster-size cross-sections for rate theory models

Damage accumulation in Cu

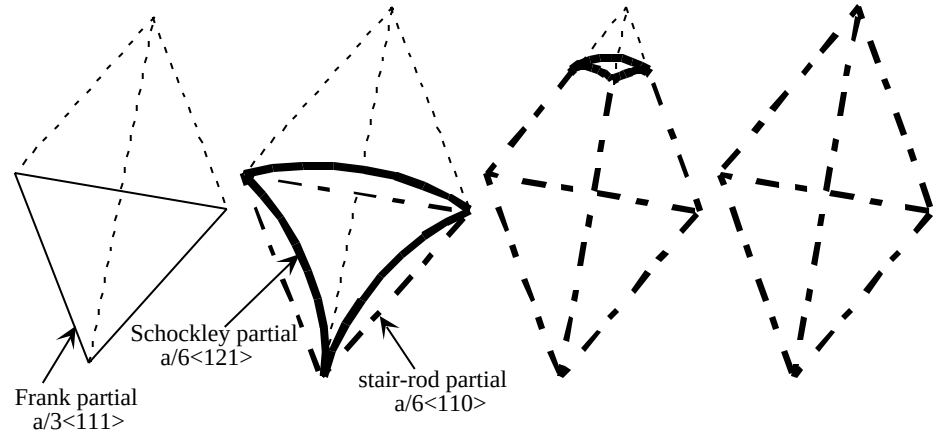
- **Experimental observations of irradiated Cu reveal that majority of defects (~90%) are stacking fault tetrahedra (SFT)**
  SFT mean size ~ 2.5 ± 0.5 nm

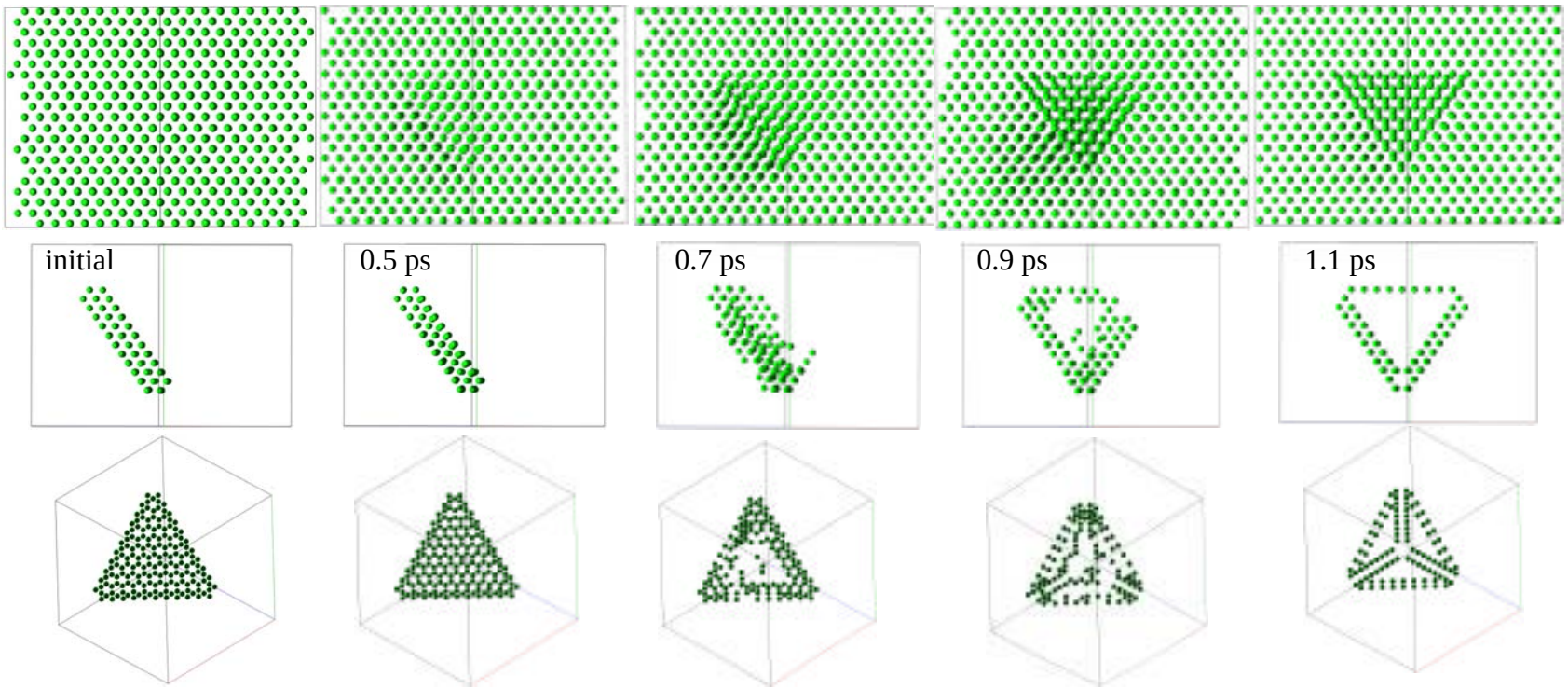
- **Coupled MD/KMC approach:**
  - MD simulations of SFT formation
  - KMC simulations of damage accumulation

- **MD simulations of dislocation - SFT interactions**

Stacking fault tetrahedra (SFT) formation

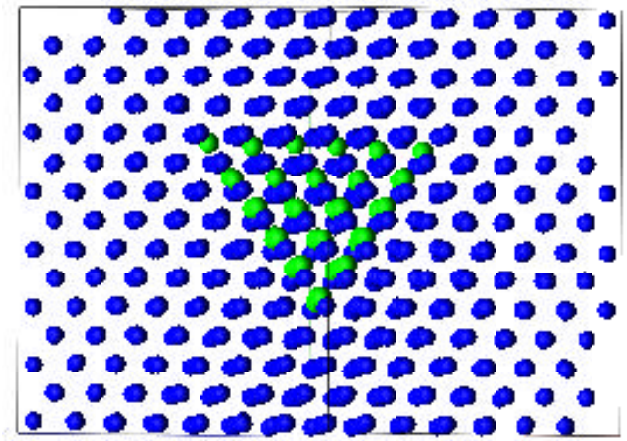
- **SFT formation mechanism in low-stacking fault energy FCC metals revealed by atomistic modeling *(EAM-type potential)***





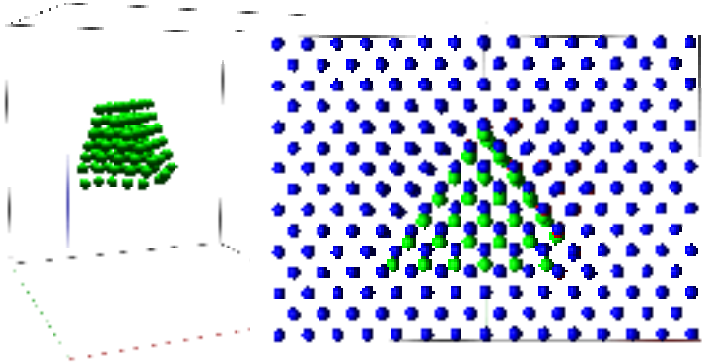
SFT formation under irradiation

Perfect SFT

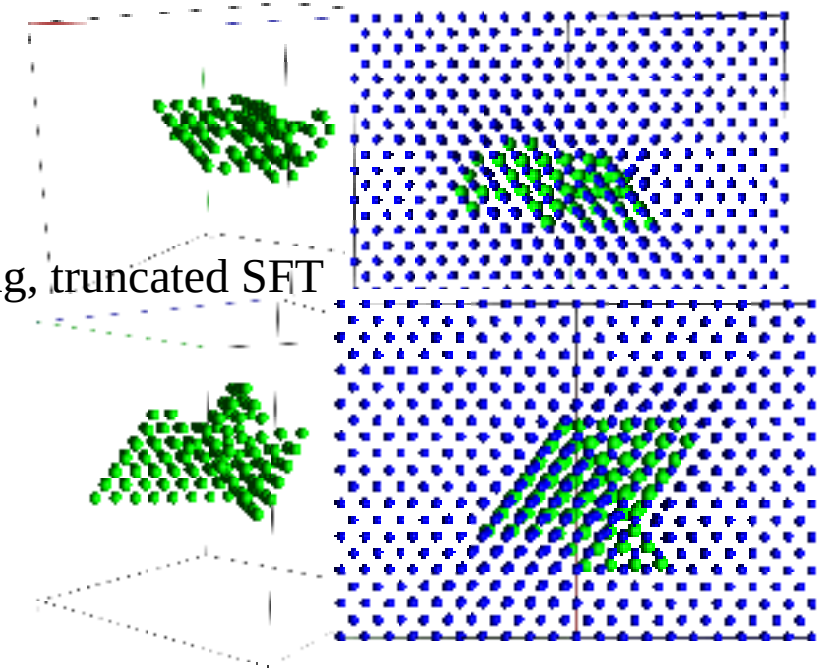


- **MD simulations of the vacancy configurations produced in high energy displacement cascades reveal truncated SFT formation**

Truncated SFT



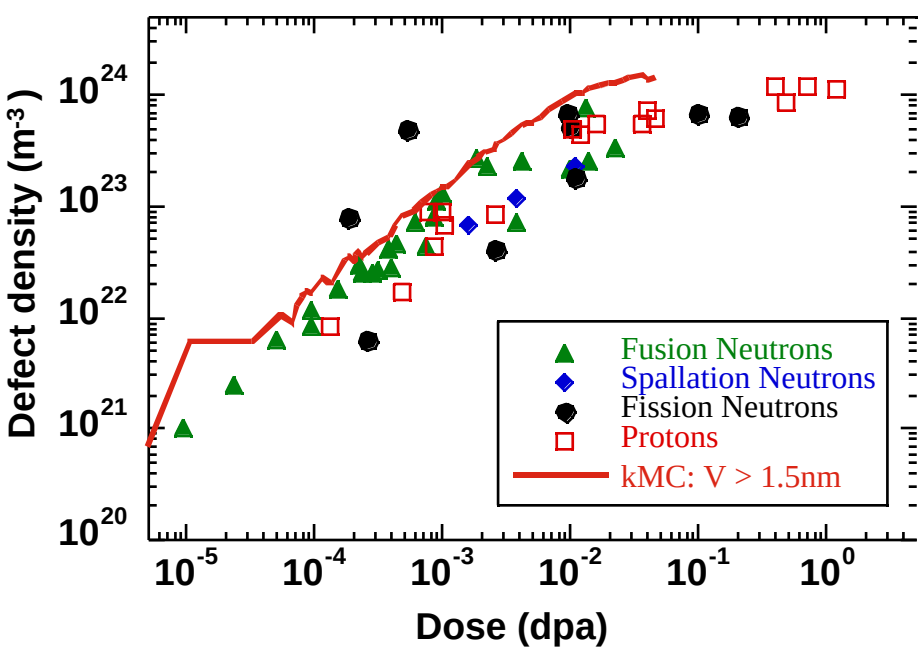
Overlapping, truncated SFT

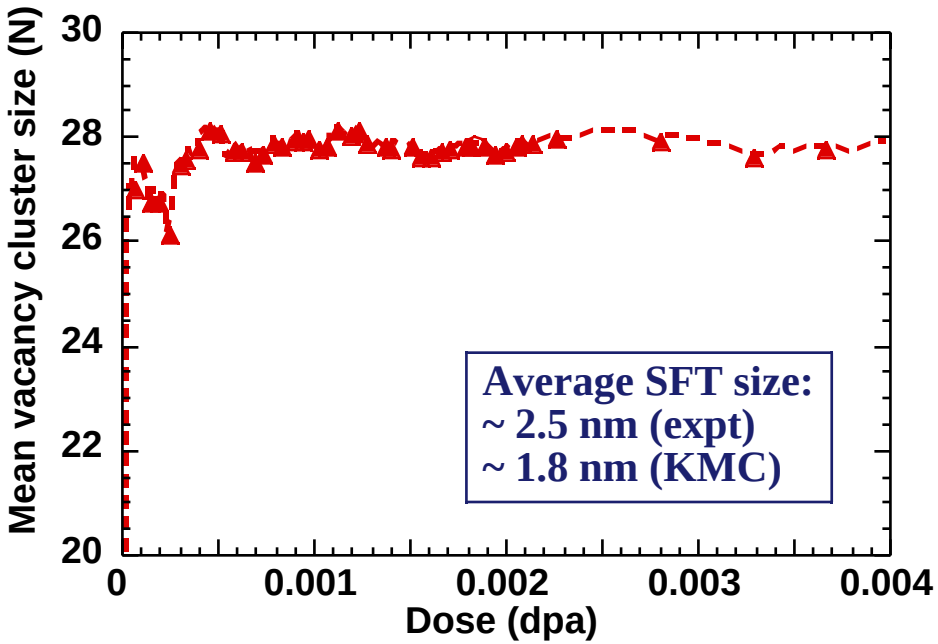


Damage accumulation in Cu

- KMC input: primary damage cascades (MD), 1-D interstitial cluster migration, SFT formation, defect cluster binding and diffusion energetics

- KMC predictions: > 90% observable defects are SFT, defect number density and mean size

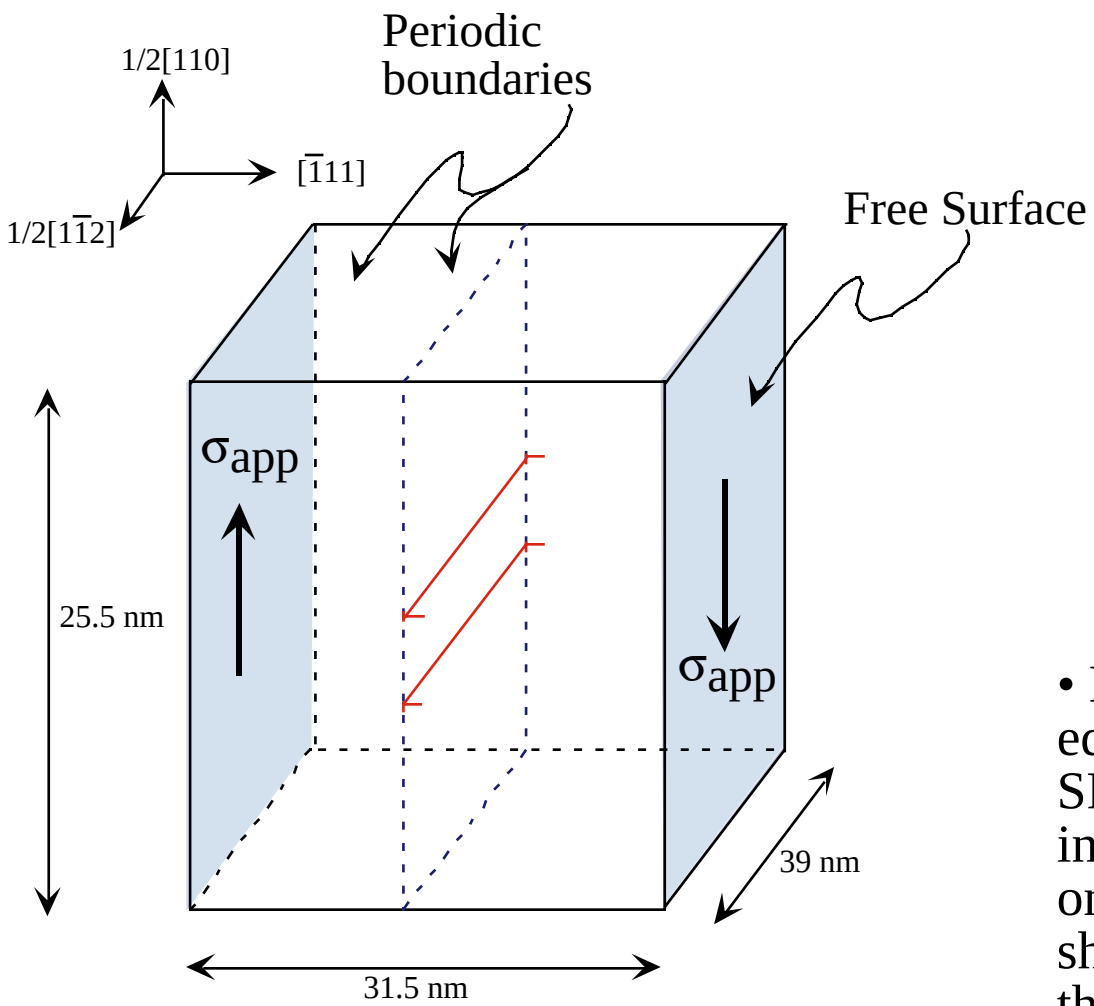




Excellent agreement between KMC predictions and experiment

Edge dislocation - SFT interaction (Cu)

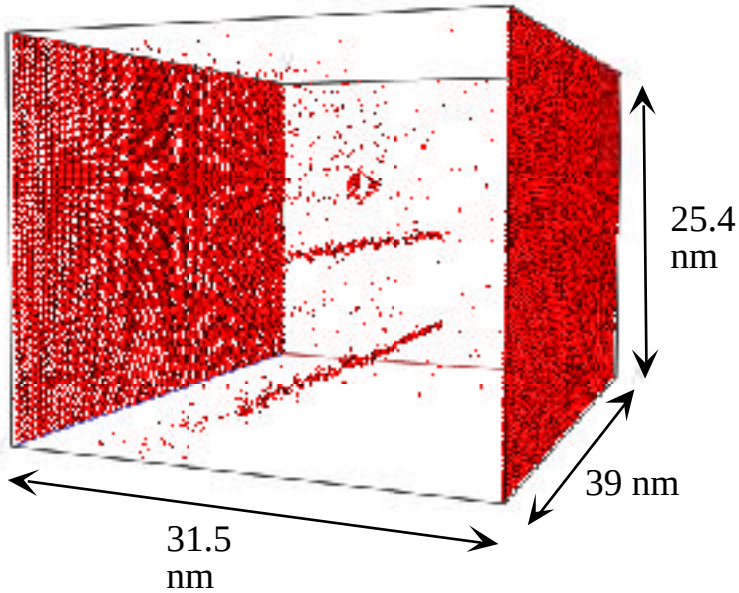
- **Atomistic (MD) simulations of individual dislocation - obstacle interactions provide fundamental understanding of radiation hardening and flow localization phenomena**

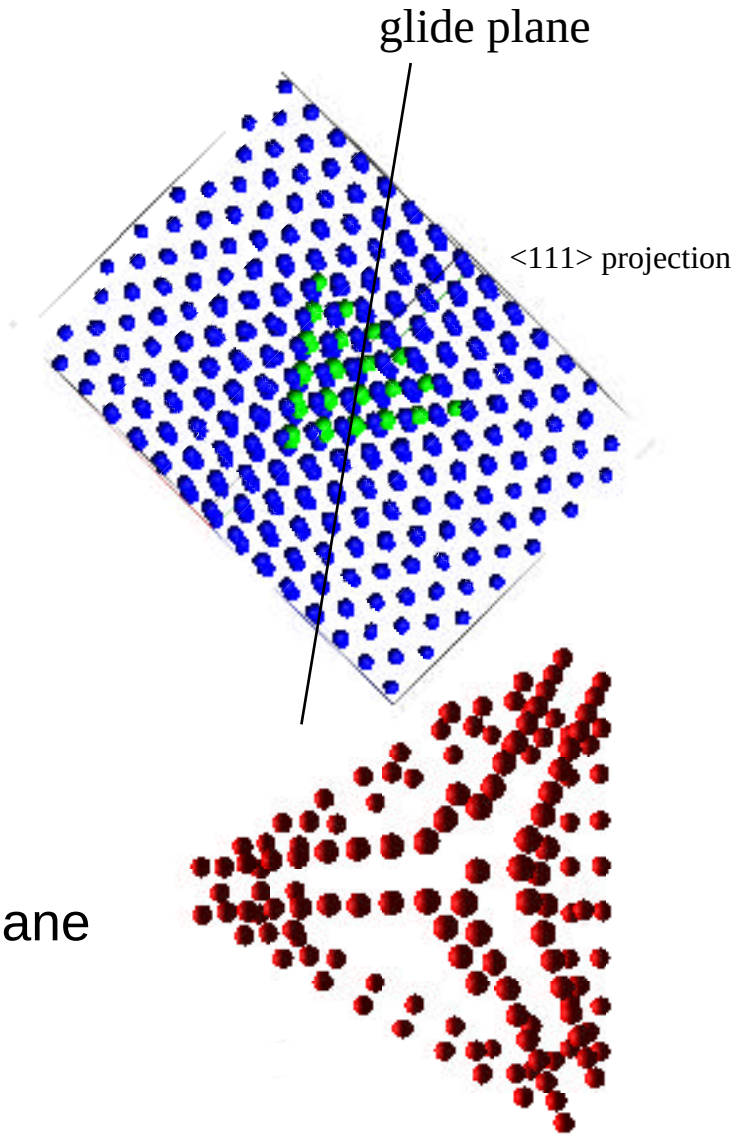


EAM Cu:	
	(10^{10} Pa)
c_{11}:	17.6
c_{12}:	12.9
c_{44}:	8.23
μ:	5.88
γ_{SFE}:	11.40 mJ/m^2

- Dislocations inserted and equilibrated at 100 K, SFT (and overlapping SFT) inserted (above, below and on the glide plane) and shear stress applied to move the dislocations

Dislocation - SFT interaction





- 39 nm line - SFT crosses the glide plane

Dislocation - SFT interaction (300 MPa)

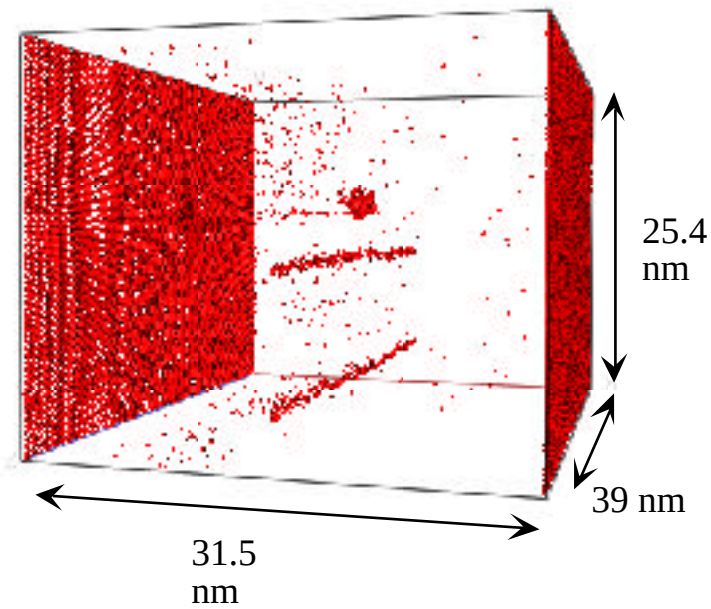
near - <111> projection

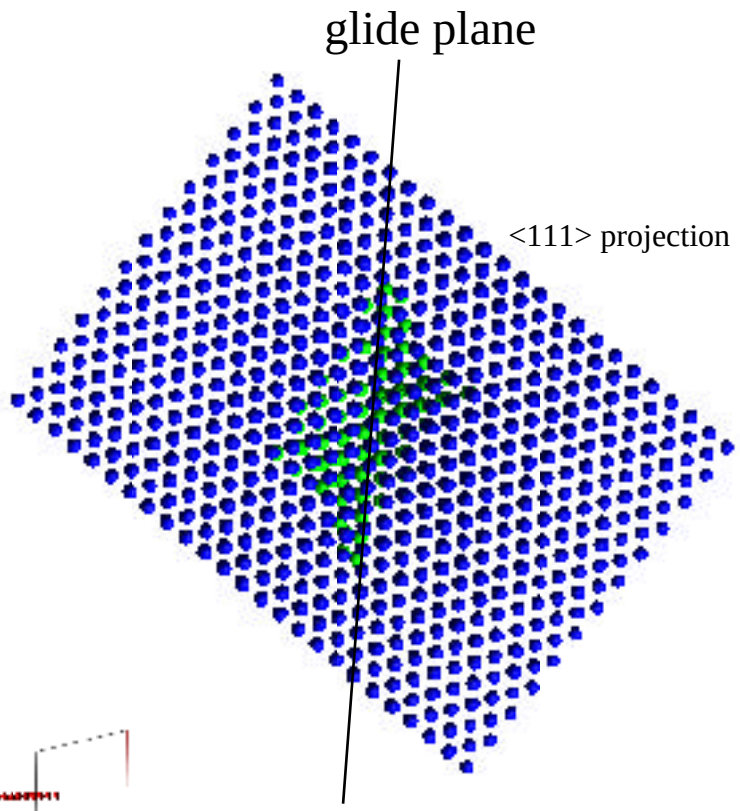
• SFT is a relatively strong obstacle $\phi \sim 80°$

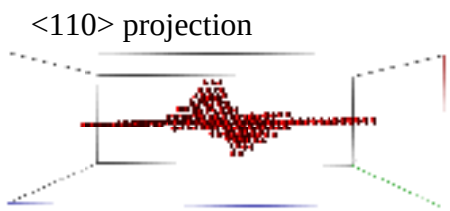
• SFT sheared but neither absorbed or destroyed

Dislocation - SFT interaction movie

Dislocation - truncated SFT interaction







- 39 nm line - overlapping, truncated SFT crosses the glide plane

Dislocation - truncated SFT (300 MPa)

near - <111> projection

- Truncated SFT is absorbed
- Vacancy absorption produces super-jog pairs
- Dislocation bows around superjogs

Dislocation - truncated SFT interaction movie

Summary

- Importance of cascade aging to damage accumulation and microstructure evolution

- Kinetic Monte Carlo provides fundamental insight into cascade aging processes, revealing
  - impact of 1-D interstitial loop on defect reaction kinetics
  - vacancy cluster formation mechanisms in Fe
    -> link (delayed cluster production cross-sections) to rate theory models
  - accumulation of SFT in Cu with constant mean size

- Molecular Dynamics simulations of dislocation-obstacle interactions provide fundamental understanding of radiation hardening and flow localization phenomena

- KMC/MD techniques are applicable to He-vacancy cluster evolution and dislocation - loop interactions relevant for fusion applications